Adaptability and "Intermediate Phases" in Randomly Connected Networks

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We consider an assembly of atoms, with a certain number of bonds between them that impose constraints on the relative positions of the atoms. If there are few bonds, the network is easily deformed: it is in the "floppy," or underconstrained, phase. If there are many bonds, any deformation requires stretching or bending bonds: this is the "rigid," or overconstrained, phase. In between these cases lies the rigidity transition. Rigidity theory, developed by Phillips [1] and Thorpe [2], has proved very successful during the last two decades in describing a variety of covalent glasses: signatures of the rigidity transition have been found by varying the composition of the glass. More recently, in a series of experiments, Boolchand et al. [3] showed that the phenomenology can be more complex than expected around the transition: they identified an intermediate phase between the floppy and rigid ones, and thus two transitions instead of one. Figure 1 provides such an example for the Si_xSe_{1-x} compound. This phase diagram with two transitions has been found now in numerous different compounds.

Thorpe et al. [4] attributed this behavior to the possibility of *self-organization* of the network; that is, the bonds are not distributed randomly, and the network can adapt itself to lower the stress due to overconstrained regions. Micoulaut and Phillips then analyzed the local and medium range structure of such self-organizing networks by growing clusters [5]. Our aim here is to provide a solvable minimal model for the intermediate phase and the two-phase transitions; the only ingredients are a network undergoing a rigidity transition, and the adaptability of the network, to avoid stress. We consider N atoms of two different types: N_1 with coordination 1 and N_3 with coordination 3. To keep the model solvable, we consider that these atoms are randomly bonded together (see Fig. 2). Without the adaptability ingredient, this system undergoes a standard rigidity transition, between a floppy and a rigid phase, when the fraction $x_3 = N_3/N$ of 3-atoms is increased where $N = N_1 + N_3$.

We now introduce the adaptability as follows. When a new bond is added to the network, it can reduce the number of degrees of freedom, or create redundancies (or both). In the presence of redundancies, some constraints cannot be fulfilled: this creates stress in the

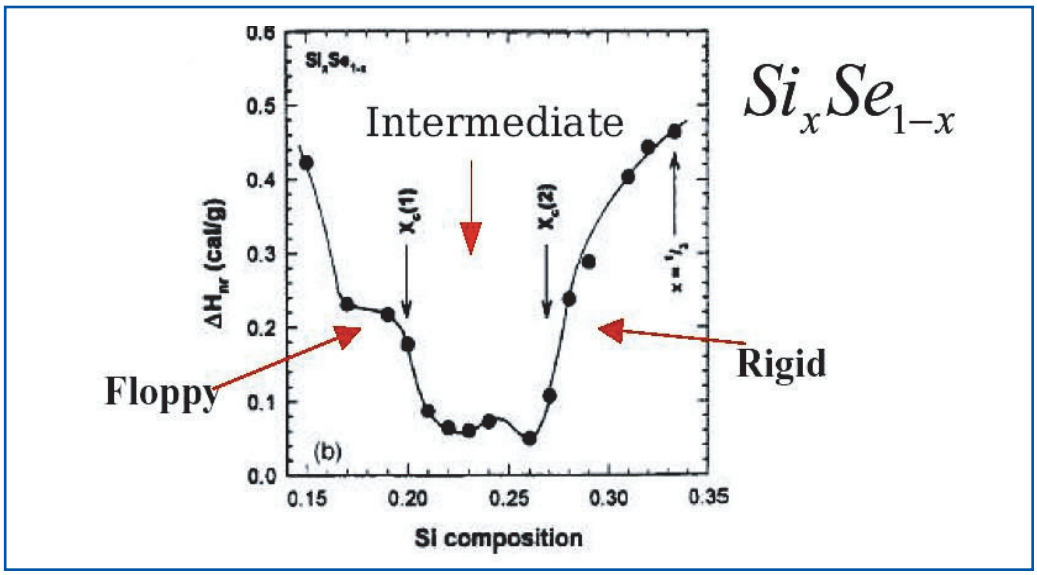

Figure 1 *— Plot of the irreversible part of the heat flow ΔH_{nr} across the glass transition for Si_xSe_{1-x} compounds, varying the Si concentration. ΔH_{nr} almost vanishes in a composition window defining the intermediate phase (experiments by Selvanathan et al. [3]).*

network and costs some energy. Thus we introduce an energy for the system defined as the number of redundant constraints in the network: $H = N_{red}$. The network now tends to adapt itself to avoid creating too many redundant constraints; however, this adaptation, pushing the network away from the completely random situation, costs entropy. A balance between the two effects is then achieved. To have a measure of how much the system adapts, or how far it is from the maximally random case, we introduce the parameter *a*, defined as the ratio of the number of bonds between two 1-atoms N_{11} and the number of bonds between two 1-atoms in the maximally random case N_{11}^*: $a = N_{11}/N_{11}^*$. Thus, any value of *a* different from one denotes some organization in the network. Analytical calculations and Monte Carlo simulations now show three different phases, see Fig. 3.

Here we have augmented a standard rigidity model with an additional ingredient: the possibility for the network to adapt, in order to avoid stress. We see that these very simple ingredients are already sufficient to produce an intermediate phase and the two-phase transitions, reproducing the experimental phase diagram. This suggests that, beyond the case of rigidity and its application to covalent glasses, this type of intermediate phase could be found in other contexts, like K-satisfiability and other combinatorial optimization problems in computer science [7].

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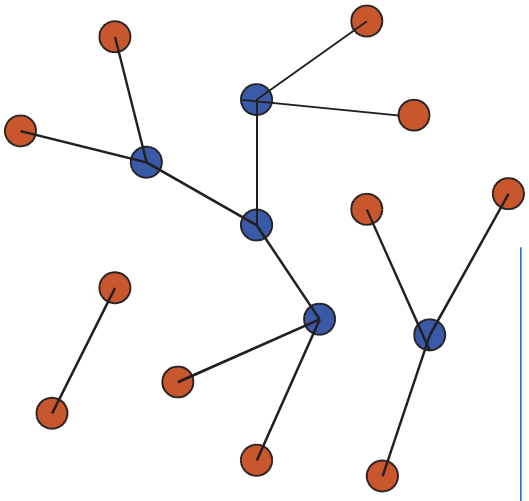

***Figure 2—** Example of a network formed with 3-atoms (blue) and 1-atoms (red).*

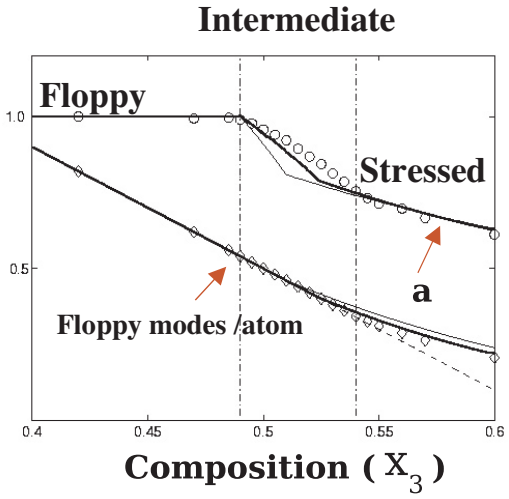

***Figure 3—** Rigidity transition with adaptability. Number of floppy modes and parameter a as a function of the composition. The lines are two analytical calculations, the solid line taking more accurately into account the correlations in the network. Symbols are Monte Carlo results.*